

Distiller Processing settings for TripleTof 5600

```
<?xml version="1.0" encoding="UTF-8"?>
<processingOptions xmlns="http://www.matrixscience.com/xmlns/schema/mdro_proc_opts_1"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" majorVersion="1" minorVersion="4"
xsi:schemaLocation="http://www.matrixscience.com/xmlns/schema/mdro_proc_opts_1
http://www.matrixscience.com/xmlns/schema/mdro_proc_opts_1/mdro_proc_opts_1.xsd">
  <scanOptions level="1">
    <preferredSpectrumFormat>0</preferredSpectrumFormat>
    <uncentroidingHalfWidth>0.2</uncentroidingHalfWidth>
    <uncentroidingPointsPerDa>20</uncentroidingPointsPerDa>
    <alwaysUncentroid>true</alwaysUncentroid>
    <regriddingPointsPerDa>20</regriddingPointsPerDa>
    <aggregationMethod>sum</aggregationMethod>
    <minPeakCount>1</minPeakCount>
    <minPeakCharge>1</minPeakCharge>
    <maxPeakCharge>5</maxPeakCharge>
  </scanOptions>
  <scanOptions level="2">
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    <uncentroidingPointsPerDa>20</uncentroidingPointsPerDa>
    <alwaysUncentroid>true</alwaysUncentroid>
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    <aggregationMethod>timedomain</aggregationMethod>
    <minPeakCount>10</minPeakCount>
    <minPeakCharge>1</minPeakCharge>
    <maxPeakCharge>2</maxPeakCharge>
    <usePrecursorAsMaxCharge>false</usePrecursorAsMaxCharge>
    <precursorChargeSources>
      <surveyScan priority="0"/>
      <file priority="1"/>
    </precursorChargeSources>
    <precursorDefaultCharges>2 3</precursorDefaultCharges>
    <redeterminePrecursorMZ>true</redeterminePrecursorMZ>
    <precursorMZTolerance>2.1</precursorMZTolerance>
    <ignoreSingleChargedPrecursor>false</ignoreSingleChargedPrecursor>
  </scanOptions>
  <timeDomainOptions>
    <minPrecursorMass>700</minPrecursorMass>
    <maxPrecursorMass>16000</maxPrecursorMass>
    <precursorGroupingTolerance>0.1</precursorGroupingTolerance>
    <maxIntermediateTime>0</maxIntermediateTime>
    <maxIntermediateScans>1</maxIntermediateScans>
    <useInterScanCount>false</useInterScanCount>
    <minScansInGroup>1</minScansInGroup>
    <collapseMSn>false</collapseMSn>
  </timeDomainOptions>
  <peakSelectionOptions level="1">
    <filteringThreshold>0.7</filteringThreshold>
```

```
<minFilteringPeakMZ>50</minFilteringPeakMZ>
<maxFilteringPeakMZ>100000</maxFilteringPeakMZ>
<filteringMinSNRatio>2</filteringMinSNRatio>
<minPeakWidth>0.005</minPeakWidth>
<expectedPeakWidth>0.03</expectedPeakWidth>
<maxPeakWidth>0.1</maxPeakWidth>
<maxIterations>500</maxIterations>
<rejectWidthOutliers>>false</rejectWidthOutliers>
<baselineCorrection>>false</baselineCorrection>
<baselineSubtractMethod>0</baselineSubtractMethod>
<peakFitMethod>0</peakFitMethod>
<isotopeEnvelopeMode>0</isotopeEnvelopeMode>
<isotopePeakIntensities/>
<singlePeakCharge>1</singlePeakCharge>
<singlePeakWindow>>false</singlePeakWindow>
<minSglPeakWindowMZ>112.5</minSglPeakWindowMZ>
<maxSglPeakWindowMZ>121.5</maxSglPeakWindowMZ>
</peakSelectionOptions>
<peakSelectionOptions level="2">
  <filteringThreshold>0.7</filteringThreshold>
  <minFilteringPeakMZ>50</minFilteringPeakMZ>
  <maxFilteringPeakMZ>100000</maxFilteringPeakMZ>
  <filteringMinSNRatio>2</filteringMinSNRatio>
  <minPeakWidth>0.005</minPeakWidth>
  <expectedPeakWidth>0.03</expectedPeakWidth>
  <maxPeakWidth>0.1</maxPeakWidth>
  <maxIterations>500</maxIterations>
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  <baselineCorrection>>false</baselineCorrection>
  <baselineSubtractMethod>0</baselineSubtractMethod>
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  <isotopeEnvelopeMode>0</isotopeEnvelopeMode>
  <isotopePeakIntensities/>
  <singlePeakCharge>1</singlePeakCharge>
  <singlePeakWindow>>false</singlePeakWindow>
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</peakSelectionOptions>
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```

Mascot Average Quantitation Method

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<method constrain_search="false" description="Average protocol" min_num_peptides="2" name="TFD -
Average [MD]" protein_ratio_type="average" report_detail="true" require_bold_red="true"
show_sub_sets="0.00" sig_threshold_value="0.01">
  <quality isolated_precursor="false" isolated_precursor_threshold="0.7" min_precursor_charge="1"
minimum_a1="0.0" pep_threshold_type="at least homology" unique_pepseq="false"/>
  <integration all_charge_states="false" all_charge_states_threshold="0.20" allow_elution_shift="false"
elution_profile_correlation_threshold="999" elution_time_delta="0.0" elution_time_delta_unit="seconds"
matched_rho="0.8" method="simpsons" simple_ratio="false" source="survey" xic_max_width="250"
xic_smoothing="3" xic_threshold="0.3"/>
  <protocol>
    <average num_peptides="3" reference_amount="1.0" selection="unique_sequence"/>
  </protocol>
</method>
```